



Glenn T. Seaborg Center Seminar

Polymerization Reactions in Ionized Clusters of Acetylene and its Derivatives: Evidence for the Formation of the Benzene and Triphenyl Benzene Radical Ions

Paul O. Momoh

*Department of Chemistry
Virginia Commonwealth University
Richmond, Virginia 23284-2006*

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Building 70A, Room 3377**

Gas phase and cluster studies provide unique opportunities to quantitatively study interesting polymerization processes. One of such processes is the reaction of acetylene and acetylene-type molecules to form polymers such as polycyclic aromatic hydrocarbons (PAHs). PAHs, a major constituent in combustion processes, are believed to be pervasive in space and could be a source of unidentified diffused infrared bands (DIBs).^{1,2} Ambient conditions of infant/aging stars and dense interstellar clouds create conditions amenable to polymerization processes. In addition, PAHs with imbedded nitrogen atoms (PANHs) have also been discovered in space and there is growing interest in elucidating the mechanism for the incorporation of nitrogen into cyclic rings. Such processes may provide insights into the primordial synthesis of biologically significant precursors such as amino acids and peptides.³ In this presentation, evidence is provided by way of collision induced dissociation (CID), reduced mobility (K_0)/collision cross section (Ω), thermochemical, and kinetic measurements, as well as theoretical calculations for the formation of the benzene ($C_6H_6^{*+}$) and triphenyl benzene ($C_{24}H_{18}^{*+}$) radical ions following the electron impact ionization of neutral clusters of acetylene (C_2H_2)_n⁺ and phenylacetylene (C_8H_6)_n⁺ respectively. Our results indicate that the measured Ω (300K) values for the mass selected acetylene, (C_2H_2)₃⁺, and phenylacetylene, (C_8H_6)₃⁺, trimers are $47.4 \pm 1.4 \text{ \AA}^2$ and $120.6 \pm 2.1 \text{ \AA}^2$, respectively.⁴ These values are in excellent agreement with the Ω values for the benzene⁵ and triphenyl benzene radical ions. In addition, the (C_2H_2)₃⁺ and (C_8H_6)₃⁺ ions showed similar dissociation and hydration behaviors as the benzene⁶ and triphenyl benzene ions, respectively. The application of the ion-mobility technique for separating and analyzing electronic states of transition metal cations, "electronic-state chromatography," is also briefly presented.

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Host: John K Gibson (510) 486-7891 JKGibson@lbl.gov Admin. Assistant: Catherine Mendez (510) 486-5587

Ernest Orlando Lawrence Berkeley National Laboratory

One Cyclotron Road | Berkeley, California 94720

| Tel: 510.486.4000